Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 22 NOV 2004 HIGHEST RN 786612-66-6
DICTIONARY FILE UPDATES: 22 NOV 2004 HIGHEST RN 786612-66-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

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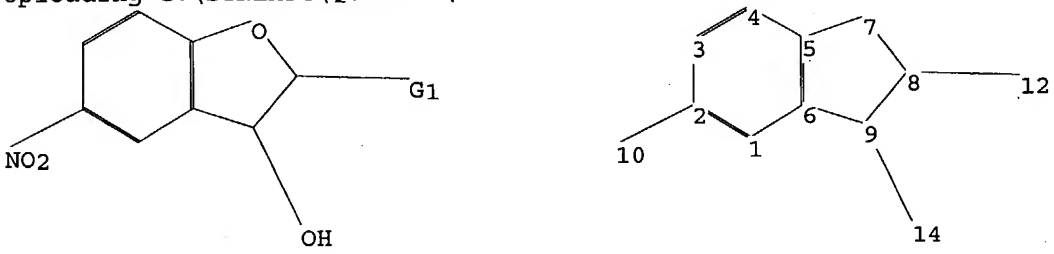


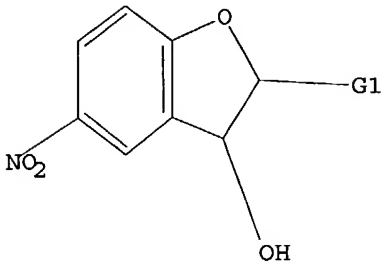
chain nodes :
10 12 14
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
2-10 8-12 9-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
8-12 9-14
exact bonds :
2-10 5-7 6-9 7-8 8-9
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G1:H,C

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 12:CLASS 14:CLASS

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



G1 H,C

Structure attributes must be viewed using STN Express query preparation.

=> s l1 ful
FULL SEARCH INITIATED 13:37:22 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 855 TO ITERATE

100.0% PROCESSED 855 ITERATIONS 20 ANSWERS
SEARCH TIME: 00.00.01

L2 20 SEA SSS FUL L1

=> fil caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION

FULL ESTIMATED COST 155.42 155.63

FILE 'CAPLUS' ENTERED AT 13:37:27 ON 23 NOV 2004
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FILE COVERS 1907 - 23 Nov 2004 VOL 141 ISS 22
FILE LAST UPDATED: 22 Nov 2004 (20041122/ED)

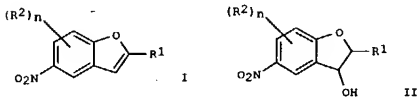
This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l2
L3 7 L2

L3 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2004:142849 CAPLUS
DOCUMENT NUMBER: 140:181316
TITLE: Process for the preparation of 5-nitrobenzofurans by dehydration of 5-nitro-2,3-dihydrobenzofuran-3-ols in the presence of protic acids or hydroxides
INVENTOR(S): Magerlein, Wolfgang
PATENT ASSIGNEE(S): Germany
SOURCE: U.S. Pat. Appl. Publ., 11 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

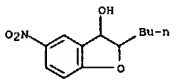
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004034220	A1	20040219	US 2003-642947	20030818
DE 10237819	A1	20040304	DE 2002-10237819	20020819
EP 1394155	A2	20040303	EP 2003-17811	20030805
EP 1394155	A3	20040324		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1485323	A	20040331	CN 2003-154803	20030819
PRIORITY APPLN. INFO.:			DE 2002-10237819 A	20020819

OTHER SOURCE(S): MARPAT 140:181316
GI

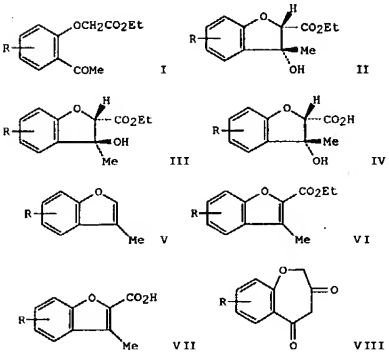


AB The invention relates to a process for preparation 5-nitrobenzofurans I by dehydration of 5-nitro-2,3-dihydrobenzofuran-3-ols II in the presence of protic acids or hydroxides [wherein R1 = H, alkyl; R2 = independently F, Cl, br, I, alkyl, OH and derivs., NH2 and derivs., CONH2 and derivs.; n = 0-3; or when n= 2, 3 it is possible that R2CCR2 = (un)substituted ring; with the proviso of 2-(n-butyl)-5-nitrobenzofuran be excluded] were prepared as new active compds. for treating cardiac arrhythmias. The advantages include low-cost, stable and easily obtainable precursors, higher product yields, and minimization of waste. For example, 2-(n-butyl)-5-nitrobenzofuran was prepared, in 80% yield, by dehydration of 2-(n-butyl)-5-nitro-2,3-dihydrobenzofuran-3-ol (III) in EtOH in the presence of concentrated H2SO4 at reflux for 4 h. III was prepared in 6 steps by O-alkylation of Me salicylate with methyl-2-bromohexanoate,
)

L3 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
NaOH-hydrolysis, cyclizing decarboxylation of 2-(1-carboxypentoxy)benzoic acid, HCl-hydrolysis, nitration in the presence of HNO3/H2SO4, and redn. with NaBH4 in ethanol.
IT **658053-39-5P**, 2-(n-Butyl)-5-nitro-2,3-dihydrobenzofuran-3-ol
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; process for preparation of 5-nitrobenzofurans by dehydration of 5-nitro-2,3-dihydrobenzofuran-3-ols in the presence of protic acids or hydroxides)
RN 658053-39-5 CAPLUS
CN 3-Benzofuranol, 2-butyl-2,3-dihydro-5-nitro- (9CI) (CA INDEX NAME)



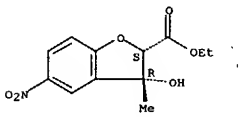
L3 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1992:448242 CAPLUS
DOCUMENT NUMBER: 117:48242
TITLE: Benzofuran derivatives. Part 4. Synthesis of benzofurans and 2,3,4,5-tetrahydro-1-benzoxepin-3,5-diones
AUTHOR(S): Suzuki, Tsuneo; Tanemura, Kiyoshi; Horaguchi, Takaaki;
Shimizu, Takahachi; Sakakibara, Tohru
CORPORATE SOURCE: Sch. Den. Niigata, Nippon Dent. Univ., Hamaura, 951, Japan
SOURCE: Journal of Heterocyclic Chemistry (1992), 29(2), 423-9
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB By treatment of Et 4- or 5-substituted 2-acetylphenoxyacetates I (R = 4-Me, H, 5-Cl, etc.) with potassium hydroxide in dry dioxane, benzofurans II-VII and 2,3,4,5-tetrahydro-1-benzoxepin-3,5-diones VIII were obtained. The relative yields of benzofurans II-VII and 2,3,4,5-tetrahydro-1-benzoxepin-3,5-diones VIII varied with the types of 4- or 5-substituents. The electron-donating 4-methoxy group favored the formation of benzoxepins. On the other hand, electron-withdrawing substituents such as the 4-nitro group favored the formation of benzofurans. When esters I were treated with sodium amide, 2,3-dihydrobenzofurans II were obtained exclusively regardless of 4- or 5-substituents.

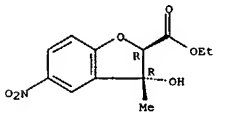
L3 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
IT **104862-17-1P 104862-21-7P 104862-25-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 104862-17-1 CAPLUS
CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-3-methyl-5-nitro-, ethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



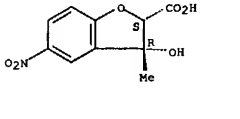
RN 104862-21-7 CAPLUS
CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-3-methyl-5-nitro-, ethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

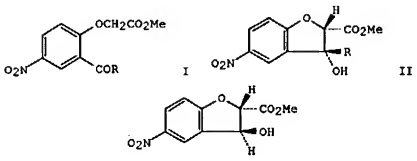


RN 104862-25-1 CAPLUS
CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-3-methyl-5-nitro-, cis-
(9CI) (CA INDEX NAME)

Relative stereochemistry.



L3 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1989:94892 CAPLUS
DOCUMENT NUMBER: 110:94892
TITLE: The cyclization reaction of methyl 2-acyl-4-nitrophenoxyacetates with potassium hydroxide
AUTHOR(S): Suzuki, Tsuneo
CORPORATE SOURCE: Sch. Dent., Nippon Dent. Univ., Niigata, 951, Japan
SOURCE: Nippon Shika Daigaku Kiyo, Ippan Kyoiku-kei (1988), 17, 111-18
CODEN: NSDKDD; ISSN: 0385-1605
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I II

III

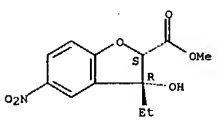
AB Cyclization of nitrophenoxyacetate I (R = H) with KOH in dioxane gave a mixture of cis- and trans-benzofurancarboxylates II (R = H) and III, resp. Similar cyclization of I (R = Me, Et, CHMe2) gave only cis products II (R = Me, Et, CHMe2).

IT **104862-29-5 104862-30-8 119197-68-1 119197-69-2 119197-70-5 119197-71-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of, with potassium hydroxide, stereochem. of)

RN 104862-29-5 CAPLUS
CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-3-methyl-5-nitro-, methyl ester, cis- (9CI) (CA INDEX NAME)

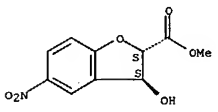
Relative stereochemistry.

L3 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



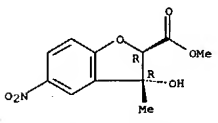
RN 119197-70-5 CAPLUS
CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-5-nitro-, methyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 119197-71-6 CAPLUS
CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-3-methyl-5-nitro-, methyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

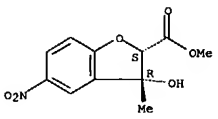


IT **104862-25-1P 104862-26-2P 119197-72-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of, with diazomethane)

RN 104862-25-1 CAPLUS
CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-3-methyl-5-nitro-, cis- (9CI) (CA INDEX NAME)

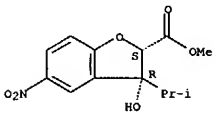
Relative stereochemistry.

L3 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



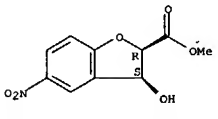
RN 104862-30-8 CAPLUS
CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-3-(1-methylethyl)-5-nitro-, methyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 119197-68-1 CAPLUS
CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-5-nitro-, methyl ester, cis- (9CI) (CA INDEX NAME)

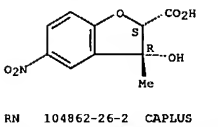
Relative stereochemistry.



RN 119197-69-2 CAPLUS
CN 2-Benzofurancarboxylic acid, 3-ethyl-2,3-dihydro-3-hydroxy-5-nitro-, methyl ester, cis- (9CI) (CA INDEX NAME)

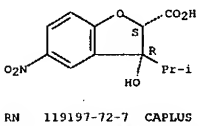
Relative stereochemistry.

L3 ANSWER 3 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



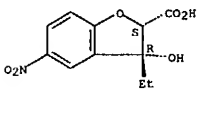
RN 104862-26-2 CAPLUS
CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-3-(1-methylethyl)-5-nitro-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 119197-72-7 CAPLUS
CN 2-Benzofurancarboxylic acid, 3-ethyl-2,3-dihydro-3-hydroxy-5-nitro-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L3 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1988:75142 CAPLUS
DOCUMENT NUMBER: 108:75142
TITLE: Benzofuran derivatives. Part 3. The reactivities of the intermediates in benzofuran synthesis
AUTHOR(S): Horaguchi, Takaaki; Matsuda, Shinichi; Tanemura, Kiyoshi; Suzuki, Tsuneo
CORPORATE SOURCE: Fac. Sci., Niigata Univ., Niigata, 950-21, Japan
SOURCE: Journal of Heterocyclic Chemistry (1987), 24(4), 965-9
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 108:75142
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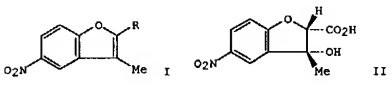
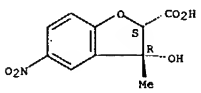


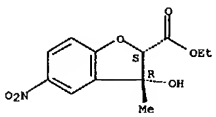
AB 3-Methyl-5-nitrobenzofuran (I, R = H) and 3-methyl-5-nitrobenzofuran-2-carboxylic acid (I, R = CO2H) were obtained by heating 2,4-Ac(NO2)C6H3OCH2CO2H with various bases in Ac2O. It appeared that 3-hydroxy-3-methyl-5-nitro-2,3-dihydrobenzofuran-2-carboxylic acid (II) was the intermediate in the benzofuran synthesis. The properties of II were examined under various conditions. Using strong bases such as Et3N in place of NaOAc, I(R = CO2H) was obtained exclusively. However, in the presence of NaOAc, I (R = H) was obtained in good yield. The reaction pathways for the formation of I (R = H, CO2H) are discussed.
IT **104862-25-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, decarboxylation, and dehydration of)
RN 104862-25-1 CAPLUS
CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-3-methyl-5-nitro-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L3 ANSWER 4 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
IT **104862-17-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, saponification, acylation, and dehydration of)
RN 104862-17-1 CAPLUS
CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-3-methyl-5-nitro-, ethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L3 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1986:590808 CAPLUS
DOCUMENT NUMBER: 105:190808
TITLE: Benzofuran derivatives. II. Synthesis of 2,3-dihydrobenzofurans from ethyl 2-acylphenoxyacetates
AUTHOR(S): Suzuki, Tsuneo
CORPORATE SOURCE: Nippon Dent. Univ. Niigata, Niigata, 951, Japan
SOURCE: Bulletin of the Chemical Society of Japan (1985), 58(10), 2821-5
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 105:190808
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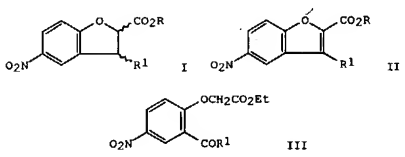
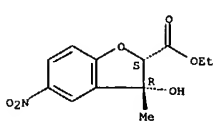


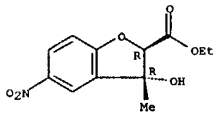
AB Benzofurancarboxylates I and II (R = H, Et; R1 = H, Me, Et, CHMe2) were obtained from the reaction of Et (2-acyl-4-nitrophenoxy)acetates III with KOH in dry dioxane. The relative ratios of the cis and trans isomers with respect to C-2 and C-3 stereochem. varied according to the structure of the acyl group. When the acyl group was acetyl, propionyl, or isobutyryl group, the cis isomers were exclusively obtained in high yields. On the other hand, a near equimol. amount of the cis and trans isomers was obtained from the reaction of 2-formyl derivs. under the same conditions.
IT **104862-17-1P 104862-21-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with potassium hydroxide)
RN 104862-17-1 CAPLUS
CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-3-methyl-5-nitro-, ethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



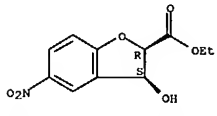
L3 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
RN 104862-21-7 CAPLUS
CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-3-methyl-5-nitro-, ethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



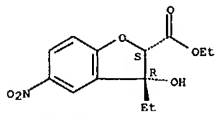
IT **104862-16-0P 104862-18-2P 104862-19-3P**
104862-20-6P 104862-25-1P 104862-26-2P
104862-29-5P 104862-30-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 104862-16-0 CAPLUS
CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-5-nitro-, ethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 104862-18-2 CAPLUS
CN 2-Benzofurancarboxylic acid, 3-ethyl-2,3-dihydro-3-hydroxy-5-nitro-, ethyl ester, cis- (9CI) (CA INDEX NAME)

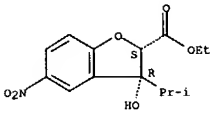
Relative stereochemistry.



RN 104862-19-3 CAPLUS
CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-3-(1-methylethyl)-5-nitro-, ethyl ester, cis- (9CI) (CA INDEX NAME)

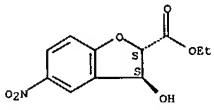
Relative stereochemistry.

L3 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



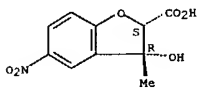
RN 104862-20-6 CAPLUS
CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-5-nitro-, ethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



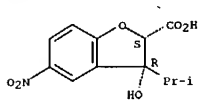
RN 104862-25-1 CAPLUS
CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-3-methyl-5-nitro-, cis-
(9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 104862-26-2 CAPLUS
CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-3-(1-methylethyl)-5-nitro-, cis- (9CI) (CA INDEX NAME)

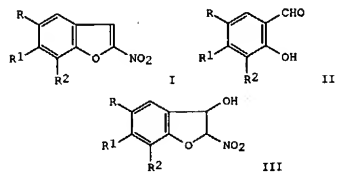
Relative stereochemistry.



RN 104862-29-5 CAPLUS

L3 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1986:552861 CAPLUS
DOCUMENT NUMBER: 105:152861
TITLE: An improved synthesis of 2-nitrobenzo[b]furans
AUTHOR(S): Tromelin, Anne; Demerseman, Pierre; Royer, Rene
CORPORATE SOURCE: Serv. Chim., Inst. Curie, Paris, F-75231, Fr.
SOURCE: Synthesis (1985), (11), 1074-6
CODEN: SYNTBF; ISSN: 0039-7881
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 105:152861
GI

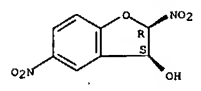


AB Ten nitrobenzofurans I (R = H, MeO, Br, NO2, MeCO, CO2Me, cyano; R1 = H, MeO; R2 = H, MeO, Br) were prepared in 2 steps by treating hydroxybenzaldehydes II with BrCH2NO2 and K2CO3 in Me2CO to give 48-97% hydroxynitrodihydrobenzofurans III which were dehydrated in refluxing Ac2O to quant. give I.

IT **104412-87-5P 104412-95-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and dehydration of)

RN 104412-87-5 CAPLUS
CN 3-Benzofuranol, 2,3-dihydro-2,5-dinitro-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

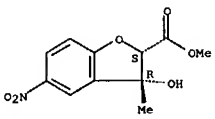


RN 104412-95-5 CAPLUS
CN 3-Benzofuranol, 2,3-dihydro-2,5-dinitro-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

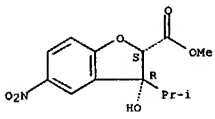
L3 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-3-methyl-5-nitro-, methyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

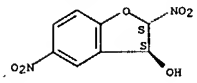


RN 104862-30-8 CAPLUS
CN 2-Benzofurancarboxylic acid, 2,3-dihydro-3-hydroxy-3-(1-methylethyl)-5-nitro-, methyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L3 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



L3 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1967:411444 CAPLUS
DOCUMENT NUMBER: 67:11444
TITLE: Benzofuranooxazines
AUTHOR(S): Hill, John; Ramage, George R.
CORPORATE SOURCE: Univ. Salford, Salford, UK
SOURCE: Journal of the Chemical Society [Section] C: Organic (1967), (8), 783-4
CODEN: JSOOAX; ISSN: 0022-4952
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 67:11444
GI For diagram(s), see printed CA Issue.
AB Syntheses of 7-acetyl-3,4-dihydro-3,6-dimethyl-2H-benzofurano-[6,5-b][1,4]oxazine (I) and related compds. are described.
IT **14742-06-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 14742-06-4 CAPLUS
CN 2-Propanone, 1-[(2-acetyl-2,3-dihydro-3-hydroxy-3-methyl-5-nitro-6-benzofuranyl)oxy]- (8CI) (CA INDEX NAME)